

Wigner Energy Generated by Isovector Pairing

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The linear term proportional to $|N - Z|$ in the nuclear symmetry energy (Wigner energy) is obtained in the framework of a model that uses isovector pairing on single particle levels from a deformed potential combined with a \bar{T}^2 interaction. The pairing correlations are calculated by numerical diagonalization of the pairing Hamiltonian acting on several levels nearest the Fermi surface. The experimental binding energies of nuclei with $N \approx Z$ are well reproduced without introducing new parameters.

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The nuclear ground state energy, $E(N, Z)$, as a function of the proton number (Z) and neutron number (N) or atomic mass number ($A = N + Z$) is very well described by the celebrated empirical mass formula (see e.g. [1])

$$E(N, Z) = E_V + E_S + E_C + E_A + E_W + E_P + E_{SHELL}. \quad (1)$$

The various terms have a clear physical meaning. The volume term, $E_V = -a_V A$, describes the constant binding energy of a nucleon in saturated nuclear matter. The surface energy, $E_S = a_S A^{2/3}$, accounts for the lack of neighbors in the surface. The term, $E_C = a_C Z^2/A^{1/3}$, is the electrostatic Coulomb energy. The (a-)symmetry energy, $E_A = a_A (N - Z)^2/A$, consists of two approximately equal contributions. The "kinetic" part accounts for the Pauli principle, which requires the nucleons to occupy higher single particle levels with increasing asymmetry $|N - Z|$. The "interaction" part originates from the difference between the proton-proton and neutron-neutron interactions and the proton-neutron interaction. The pairing energy (E_P) describes the energy gain by forming pairs of protons or neutrons. The shell energy (E_{SHELL}) is a manifestation of the level bunching around the Fermi level. The term, $E_W = a_W |N - Z|/A$, is called Wigner energy, because Wigner [2] gave a first interpretation in terms of his super multiplet theory. However its physical origin has been the subject of a long debate, which has been recently reviewed by [3]. Modern mean field approaches reproduce the ground state energies very well, except the Wigner energy, which has to be added as an ad-hoc phenomenological term (see e. g. [4]). This means that the physics behind the Wigner energy is not taken into account by present mean field theories. In this letter we demonstrate that the Wigner energy is obtained, without introducing any new parameters, by including the isovector proton-neutron pair correlations determined by numerical diagonalization of an isorotational invariant pairing Hamiltonian.

Experimentally, the coefficients a_A and a_W are not very different. As the ground state isospin (T) of most nuclei is equal to their isospin projection ($T_z = \frac{N-Z}{2}$).

The sum of the symmetry and Wigner energies is approximately proportional to $T(T+1)$. The T - dependence is suggestive, because the isospin operators obey the same SU_2 algebra as the angular momentum operators. Spontaneous breaking of the rotational symmetry by the deformed mean field leads to the appearance of rotational bands. The energies of the rotational levels are proportional to $I(I+1)$, with I being the angular momentum. The analogy between nuclear spin and isospin led Frauendorf and Sheikh [5, 6] to suggest that the $T(T+1)$ dependence of the ground state energy is a manifestation of an isorotational band.

The band appears because the isovector pair field, which is a vector, spontaneously breaks rotational symmetry in isospace. Satula and Wyss discussed the analogy of the cranking model in isospace [7, 8]. In the limit of strong symmetry breaking, simply the isorotational energy $T(T+1)/2\Theta$ is added to the intrinsic energy of the symmetry breaking mean field, the orientation of which can be taken such that the proton-neutron pair field is zero [5, 6]. Refs. [9] and [10] used this simple limit for successfully interpreting the excitation spectra of nuclei with $N \approx Z$. Applying the Mean Field and Random Phase Approximation to an isorotational invariant isovector pairing interaction, Neergård has reproduced the experimental observation $a_A \approx a_W$ [3, 11, 12]. The virtue of such an approach is that the Wigner energy appears without introducing any new parameter, because the strength of the proton-neutron pair correlation is fixed by the isorotational invariance of the isovector pairing Hamiltonian. Both approaches only work well when the isorotational symmetry is substantially broken by the isovector pair field. However, this not always the case of the medium mass nuclides, where the Wigner energy is seen to vary. For this reason, we take the pair correlation into account by numerically diagonalizing the isovector pair Hamiltonian within a configuration space spanned by seven single particle levels nearest the Fermi surface.

As a starting point we assume that the isospin mixing caused by the Coulomb interaction can be neglected. Ref. [13] estimates the admixture of components with

$T > T_z$ to the ground state to be of the order of 0.3 % for $A \sim 70$. With this assumption, the Coulomb energy can be separated from the energy caused by the strong interaction. Following [14] (and earlier work cited therein) we subtract the Coulomb energy from the experimental energies and compare the resulting energies with our model. The Myers-Swiiatecki expression for E_C [15] was used to fit the Coulomb energy difference ΔE_C between the experimental binding energies [16] of 75 pairs of even-A mirror nuclei mirror nuclei for $20 \leq A \leq 100$. We find that:

$$\frac{\Delta E_C}{\Delta Z} = 0.6967A^{2/3} - 0.8027[MeV], \quad (2)$$

which is comparable to previous fits (see e.g. [17]). After generalizing the restriction for mirror nuclei, the resulting expression for the Coulomb energy is determined:

$$E_C = 0.697 \frac{Z^2}{A^{1/3}} - 0.240 \frac{Z^2}{A} - 1.064 \frac{Z^{4/3}}{A^{1/3}} [MeV]. \quad (3)$$

In the following we use "experimental strong interaction energies" defined by $E_S = E_{Exp}(N, Z) - E_C(N, Z)$.

In accordance with the concept of isorotational bands, we write the energy of an isobaric chain ($A = Z + N = \text{const}$) in the form

$$E(N, Z) = E_{int} + \frac{T(T + X)}{2\Theta}, \quad T = |T_z| = \frac{|N - Z|}{2}, \quad (4)$$

where, E_{int} is the energy of the intrinsic ($N = Z$) configuration. As discussed in [5, 6], the ordinary BCS ground state without proton-neutron pairs is a legitimate intrinsic state. It is a mixture of only even N and Z , which implies that T_z must be even if $A/2$ is even or T_z must be odd if $A/2$ is odd. Hence the ground state isorotational bands of even-even nuclei are composed of even values of $T = T_z$ if $A/2$ is even and odd values of $T = T_z$ if $A/2$ is odd. The term $1/2\Theta$ is a combination of the coefficient a_S of the symmetry energy and a contribution from the shell energy $E_{SHELL}(Z, N)$, which depends on T_z . Likewise, X/Θ is a combination related to the coefficient a_W of the Wigner energy, which also contains a contribution from E_{SHELL} . We introduce the experimental isorotational frequency

$$\omega(T + 1) = \frac{E(T + 2) - E(T)}{2} = \frac{T + 1 + X}{\Theta}. \quad (5)$$

The slope and intercept with the ω -axis determine $1/\Theta$ and X . We take the experimental ground state energies of the three nuclei $T_z = 0, 2, 4$ if $A/2$ is even and of $T_z = 1, 3, 5$ if $A/2$ is odd and calculate two points of $\omega(T)$ by means of Eqn. 5. Note that this is just a recombination of the experimental ground state energies, which aims at exposing the the Wigner energy. Figs. 2 and 3 show the experimental values of $1/\Theta$ and X , where the experimental binding energies are taken from the most recent mass

evaluation from [16]. The small error bars for the lower mass region are primarily caused by the uncertainty in the spherical Coulomb energy fit. The large error bars in the $A > 80$ region are mainly caused by the error in binding energy of the nucleus nearest to or at $N = Z$.

A monopole isovector Hamiltonian is used to describe the pair correlated ground state,

$$H = \sum_k \epsilon_k \hat{N}_k - G \sum_{k, \tau} \hat{P}_{k, \tau}^+ \hat{P}_{k', \tau}, \quad (6)$$

$$\hat{N}_k = \hat{p}_k^+ \hat{p}_k + \hat{p}_{\bar{k}}^+ \hat{p}_{\bar{k}} + \hat{n}_k^+ \hat{n}_k + \hat{n}_{\bar{k}}^+ \hat{n}_{\bar{k}}, \quad (7)$$

$$\hat{P}_{k, 0}^+ = \frac{1}{\sqrt{2}} (\hat{n}_k^+ \hat{p}_{\bar{k}}^+ + \hat{p}_k^+ \hat{n}_{\bar{k}}^+), \quad (8)$$

$$\hat{P}_{k, -1}^+ = \hat{p}_k^+ \hat{p}_{\bar{k}}^+, \text{ and } \hat{P}_{k, 1}^+ = \hat{n}_k^+ \hat{n}_{\bar{k}}^+, \quad (9)$$

where \hat{p}_k^+ and \hat{n}_k^+ create a proton and a neutron, respectively, on the level k , and \bar{k} denotes the time reversed state of k . This Hamiltonian is invariant under rotations in isospace, i.e. it conserves isospin. The pairing problem is solved via matrix diagonalization for the three nuclei with $T_z = 0, 2, 4$ or $T_z = 1, 3, 5$.

As the computational complexity grows quickly with number of levels, the diagonalization is carried out within the configuration space spanned by the set of single particle energies ϵ_k centered around Fermi level of the $N = Z$ nuclide within the considered isobaric chain. The matrix is constructed by successive application of the pairing interaction onto the uncorrelated ground state, which ensures that the configuration space contains only states with $T = T_z$. Shell effects in the non-interacting levels outside of this window are accounted for by summing the single particle energies for all occupied proton and neutron levels. The single particle energies are calculated by means of the micro-macro method using a Nilsson Hamiltonian as described in Ref. [18]. For each nucleus the equilibrium deformation has been calculated. In these calculations BCS pairing was used with $\Delta_Z = 13.4 MeV/A^{1/2}$ and $\Delta_N = 12.8 MeV/A^{1/2}$ as suggested in [19], which means the deformation of the intrinsic state is found. Ref. [20] discusses this procedure in more detail. The resulting deformations are comparable with those from Ref. [21]. The single particle energies used in the diagonalization of the pairing Hamiltonian are taken as the average of the proton and neutron energies calculated by the Nilsson model at equilibrium deformation.

The pairing strength G must be adjusted to match the reduced single particle space. We use experimental staggering $2\Delta_{EEOO}(N, Z)$ between the lowest $T = 0$ states in the even-even and odd-odd $N = Z$ nuclei to determine $G(A)$.

$$2\Delta_{EEOO}(N, Z) = \quad (10)$$

$$\frac{|E(N - 1, Z - 1) - 2E(N, Z) - E(N + 1, Z + 1)|}{2}.$$

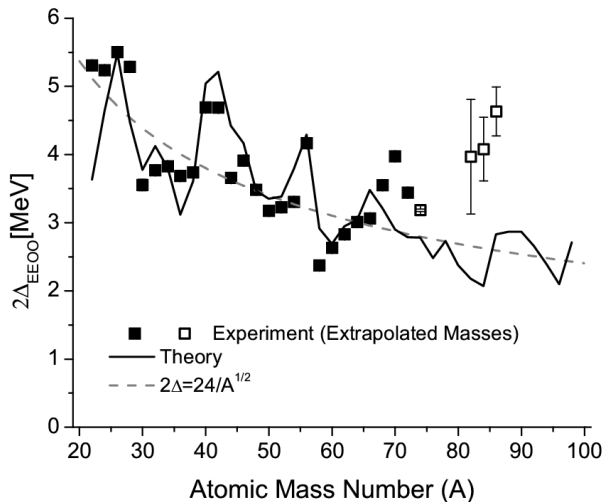


FIG. 1: The experimental even-even to odd-odd energy difference $2\Delta_{EEOO}$ compared with a seven level pairing calculation with the interaction strength (11).

The same quantity was calculated from the theoretical energies obtained by diagonalization. The lowest $T = 0$ state in the odd-odd nucleus has two-quasiparticle character (see [5]), i. e. its Fermi level is blocked. Accordingly, we remove it from the diagonalization (as discussed in [22]), which is carried out for $N = Z = A/2 - 1$. Two times the blocked single particle energy is added to the resulting energy. Fig. 1 shows that the calculations reproduce the experiment rather well using the following pairing strength:

$$G = \frac{7.63}{A^{1/2}} [MeV]. \quad (11)$$

The use of a fixed set of single particle levels within an isobaric chain only accounts for the "kinetic" part of the symmetry energy, which results in underestimating it by roughly a factor of two. Neergård suggested adding the schematic interaction $C\vec{T} \cdot \vec{T}$ in order to obtain the correct symmetry energy[11]. On the mean field level, this "symmetry interaction" generates a shift of the single particle energies by $C(N - Z)t_z$, which mimics the realistic isospin dependence of the single particle energies responsible for the interaction part of the symmetry energy (see [3, 13] for a more detailed discussion). Since T is a good quantum number, the symmetry interaction only adds $CT(T + 1)$ to the calculated energies. Fig. 2 demonstrates that

$$C = \frac{24.94}{A} [MeV] \quad (12)$$

provides an excellent reproduction of the experimental values of $1/\Theta$. The fluctuations are caused by the irregular spacing of the single particle levels, i. e. the shell structure. They are more pronounced for the spherical nuclei, which have strongly bunched levels, whereas for $62 < A < 90$ nuclear deformation generates more evenly distributed single particle levels.

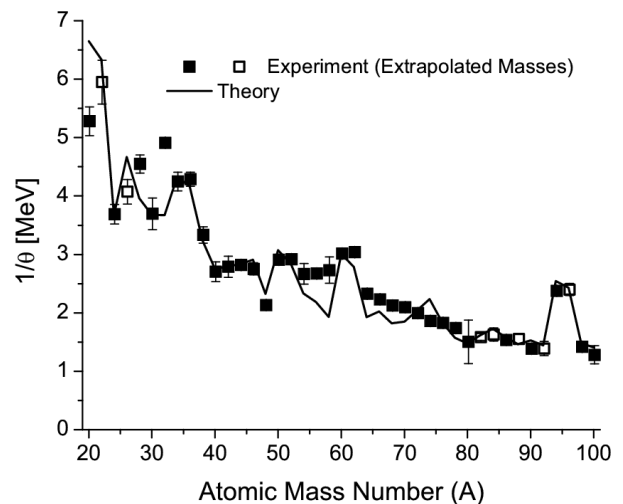


FIG. 2: The curvature of the symmetry energy ($1/\theta$) compared to experiment.

Fig. 3 demonstrates that the calculated Wigner X well reproduce the experiment. As in the case of $1/\Theta$, the fluctuations reflect the irregular level spacings. Varying the coupling constant G , we found that X approaches the strong symmetry breaking limit of 1 only for $G > 2MeV$ in the case of spherical nuclei. In the case of equidistant level it is reached for $G > 0.5MeV$. Eq.(11) gives $0.8MeV$ for $A = 80$, i. e. the pairing correlations are not strong enough to average out effects of the substantial level bunching. For most of the isobaric chains studied, the calculated X shows the same up and down variation, which is seen experimentally. The size of fluctuations of X turned out to be sensitive to the level positions near the Fermi level, which cannot be expected to be reproduced in detail by our mean field. The calculation yields X values which are too small in the region $72 \leq A \leq 92$. A possible reason for the discrepancy may be the theoretically determined deformations, which are fairly constant and small, whereas the experimental information ($B(E2, 2_1^+ \rightarrow 0_1^+)$, rotational spectra) points to large deformations for some of the considered nuclei. A supplemental calculation intended to simulate changes in deformation along an isobaric chain, as indicated by the experiment, results in X values around 2.

Odd-odd $N = Z$ nuclei with $A > 40$ often have a ground state that has $T = 1 > T_z = 0$. The inversion of the isospin order has been explained by Refs. [23] and [24]. The $T = 0$ state in the odd-odd nucleus is lifted relative to the $T = 0$ ground state of the even-even neighbors, by the two-quasiparticle excitation energy $2\Delta_{EEOO}$. The $T = 1$ state is lifted by the isorotational energy $1/\Theta$, which is somewhat smaller than $2\Delta_{EEOO}$. Fig. 4 shows that calculations fairly well reproduce energy difference between the lowest $T = 1$ and $T = 0$ states, which measures to relative strength of the pair correlation and the isorotational energies.

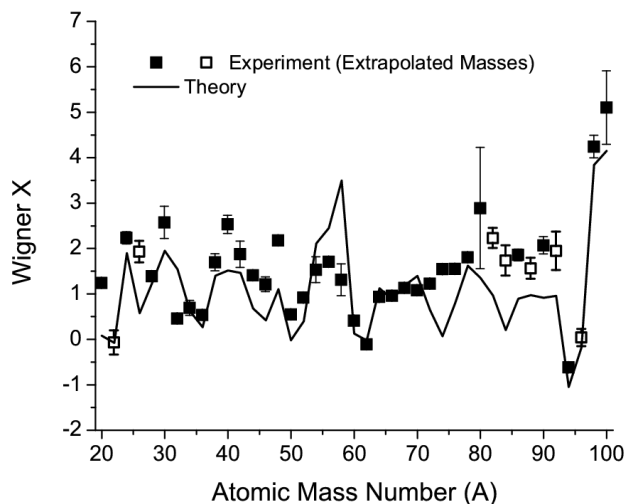


FIG. 3: The Wigner X compared to experiment.

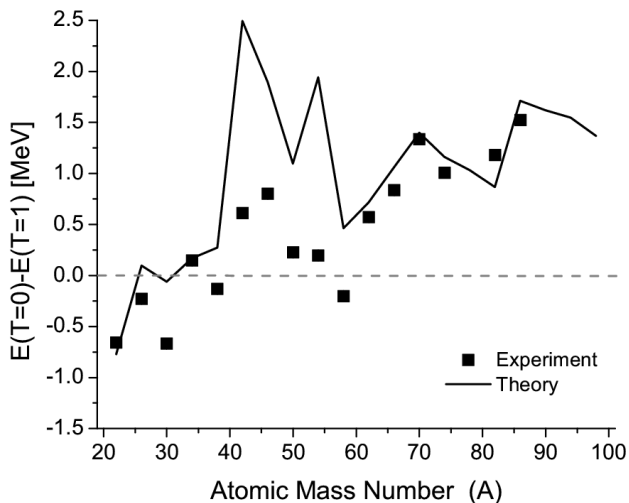


FIG. 4: Energy difference of the first $T = 0$ and first $T = 1$ states in odd-odd $N=Z$ nuclei calculation compared to [25] experiment.

We have demonstrated that a model based on single particle levels in a deformed potential, isospin conserving isovector pairing, and a schematic "symmetry" interaction proportional to \bar{T}^2 reproduces the term linear in $|N - Z|$ (Wigner energy) in the nuclear binding energy. The pairing correlations are treated exactly, not in mean field approximation, by numerical diagonalization in a space of seven single particle levels. The model does not introduce new parameters as compared to standard mean field approaches: The pairing strength is fixed by the even-even to odd-odd mass difference, and the strength of the symmetry interaction is determined by the symmetry energy. The shell structure causes strong fluctuations of the Wigner energy which are fairly well described by the model. The remaining deviations can be attributed to inaccuracies of the single particle energies. The results

seem to provide no evidence for the presence of isoscalar proton-neutron pair correlations, in contrast with claims in Refs. [7, 8]. Our results suggest that a combination of an isorotational invariant effective interaction in the particle-hole channel with isovector pairing interaction will give the Wigner energy, provided the pairing correlations are treated beyond the mean field approximation and isospin is conserved. How to accomplish this for the present standard mean field approaches remains to be studied. In a future study we will address this question by comparing our results with approximations as e. g. isospin projected mean field solutions.

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